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MAGNETIC PHASE TRANSITIONS AND GROUND STATE PROPERTIES OF MAGNE--ETC(U)

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FINAL SCIENTIFIC REPORT

AFOSR GRANT NO. 76-2981

MAGNETIC PHASE TRANSITIONS AND GROUND  
STATE PROPERTIES OF MAGNETIC CRYSTALS

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Chief, Technical Information Division

## Final Scientific Report

During the final year and one-half of this contract work continued upon ground state properties and magnetic phase transitions in magnetic crystals. A number of publications were completed which dealt with a wide range of topics related to the basic goals of this contract. A list of publications completed since the last interim report is attached at the end of this brief report.

The work has fallen into roughly four categories:

- (1) Calculation of ground state properties using standard energy band techniques
- (2) Correlation corrections to band structure predictions using techniques of many body theory
- (3) Prediction of magnetic phase transitions using the temperature dependent magnetic susceptibility
- (4) Development of practical computer codes to perform some of the complicated statistical calculations.

The progress made on the subjects is best understood by reading the published papers. A brief summary of successes and failures follows.

1. It appears that the linear-combination of atomic orbitals method of energy band theory when using a local exchange potential of the van Barth-Hedin type is quite capable of giving a good understanding of ground state properties of magnetic metals such as chromium. A major part of the effort expended over the duration of this contract was devoted to this study and resulted in several papers.

2. Accurate numerical methods of evaluating the spin and orbital susceptibilities of metals have been developed and tested successfully against well known exact results.

3. Improvements over the commonly used random-phase-approximation to the susceptibility have been made using many body theory. There has been some controversy here: the present state of understanding is given in the last publication listed below. Further numerical calculation is needed.

4. Use of the susceptibility to predict phase transitions has been justified by a calculation which successfully predicted the same results obtained from a free-energy calculation by Kimball. See the publication listed below. This is important since free-energy calculations are almost impossible for real systems.

5. A version of the analytic tetrahedron method including matrix element variation in the tetrahedron has been obtained and fully tested against well known exact results for the orbital susceptibility of the uniform electron gas.

6. The calculation of matrix elements for the susceptibility throughout the Brillouin zone for a real system using an LCAO basis has turned out to be an almost impossible job because of the storage and computer time required. An accurate method of interpolating matrix elements must be found to make possible extensive calculations for real systems.

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### Publications

D. G. Laurent, J. Callaway, J. L. Fry and N. E. Brener, "Band Structure, Fermi Surface, Compton Profile and Optical Conductivity of Paramagnetic Chromium," Phys. Rev. B 23, 497 (1981).

J. L. Fry, N. E. Brener, D. G. Laurent and J. Callaway, "Fermi Surface of Paramagnetic and Antiferromagnetic Chromium," J. Appl. Phys. 52, 2101 (1981).

N. E. Brener and J. L. Fry, "Spin Density Waves in the Uniform Electron Gas," J. Appl. Phys. 52, 1624 (1981).

P. C. Pattnaik, J. L. Fry and N. E. Brener, "Paramagnetic and Antiferromagnetic Susceptibilities of the Kimball Model of Antiferromagnetic Chromium," J. Appl. Phys. 52, 1646 (1981).

N. E. Brener, J. L. Fry and R. A. Johnson, "Matrix Elements in the Analytic Tetrahedron Method," Int. J. Quant. Chem. 15S, 459 (1980).

P. C. Pattnaik, J. L. Fry, N. E. Brener and G. Fletcher, "Use of ATM in Evaluating Spin Density," Int. J. Quant. Chem. 15S, 499 (1980).

P. C. Pattnaik, P. H. Dickinson and J. L. Fry, "Fermi-Surface: A Package to Display Perspective Drawings of Fermi Surfaces in Cubic Systems," Comp. Phys. Commun. 25, 63 (1982).

### Papers Submitted for Publication

J. L. Fry, A. V. Kugler, J. L. Thompson and N. E. Brener, "A Soluble Model of a Solid Surface" (Submitted to Int. J. of Quant. Chem.).

P. C. Pattnaik, M. S. Jay and J. L. Fry, "Accurate Numerical Methods of Evaluating Orbital Susceptibility of Solids" (Submitted to the Physical Review).

P. C. Pattnaik and J. L. Fry, "A Study of the Linear Interpolation Used in the Analytic Tetrahedron Method" (Submitted to the Physical Review).

N. E. Brener, J. L. Fry and P. C. Pattnaik, "Reply to 'Comments on a 'Time-dependent Hartree-Fock formalism for the dielectric function'" (Submitted to the Physical Review).

P. C. Pattnaik, P. H. Dickinson and J. L. Fry, "Pressure Dependence of the Fermi Surface and Nesting Wave Vector of Paramagnetic Chromium" (Submitted to the Physical Review).